Radiation Diffusion with Material-Energy Transfer Including Fusion Heat Source

Dan Shumaker, Carol Woodward, and Peter Brown

Center for Applied Scientific Computing

LLNL

UCRL-PRES-154623

Work performed under the auspices of the U. S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48

Material energy source term added to two different systems

The fusion heat source is model by a new term which depends on the material temperature to the fifth power. This is a good model for the deuterium tritium fusion reaction rate at low temperatures, (less than a few Kev).

$$energy\ source = e_r\ \sigma_v\ F^2\ T_M^5$$

- Fusion source added to two different systems

1. **Radiation diffusion equation coupled to material energy equation: Source term with predetermined time dependence of fuel density is added to the material energy equation.**
2. **Time dependence of fuel density computed by an additional equation describing the evolution of fuel density.**

System of Equations, Evolution of Radiation and Material Energy

Radiation Energy

$$\frac{\partial E_R}{\partial t} = \nabla \cdot \left(\frac{c \, \nabla E_R}{3 \rho \kappa_R (T_R) + \frac{\left\| \nabla E_R \right\|}{E_R}} \right) + c \rho \kappa_P (T_M) \cdot (a T_M^4 - E_R)$$

Material Energy

$$\frac{\partial E_M}{\partial t} = -c \; \rho \, \kappa_P (T_M) \cdot (a \, T_M^4 - E_R) + h_t(t) \;\; e_r \; \sigma_v \; F(x)^2 \; T_M^5$$

Solution Methods

- **Time integration is done with the CVODE ODE solver**
- **Implicit BDF methods**
- **Variable order (up to 5) and variable step size**
- **An inexact Newton-Krylov method is used to solve the implicit systems**
- **Schur complement Preconditioner**

The semi-implicit method linearizes the system

- Opacities are lagged in time

$$\frac{E_R^{n+1} - E_R^n}{\Delta t} = L(E_R^n)E_R^{n+1} + K(T_M^n)\left(a(T_M^{n+1})^4 - E_R^{n+1}\right)$$

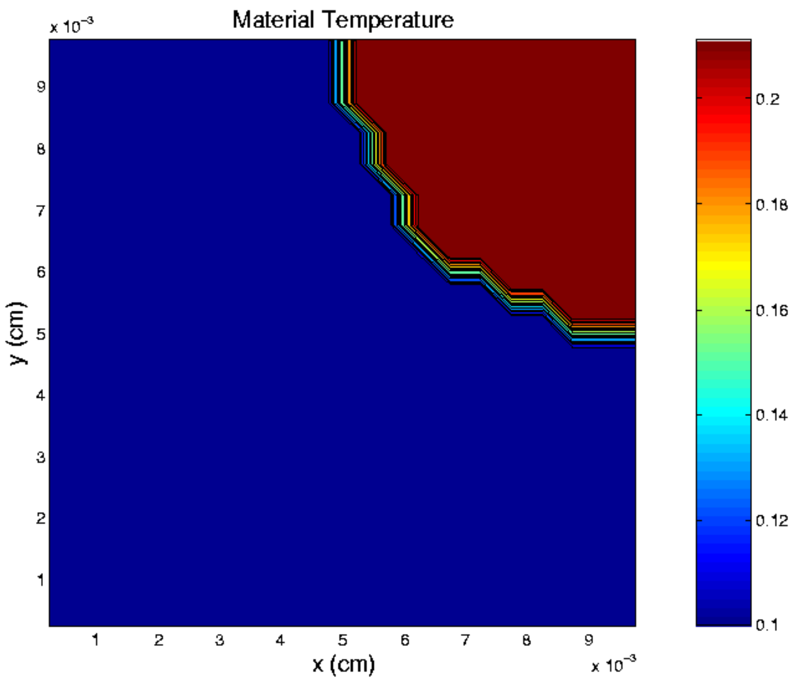
$$\frac{E_M^{n+1} - E_M^n}{\Delta t} = -K(T_M^n)\left(a(T_M^{n+1})^4 - E_R^{n+1}\right) + e_r \sigma_v h_t(t)(T_M^{n+1})^5$$

- Linearize coupling terms with:

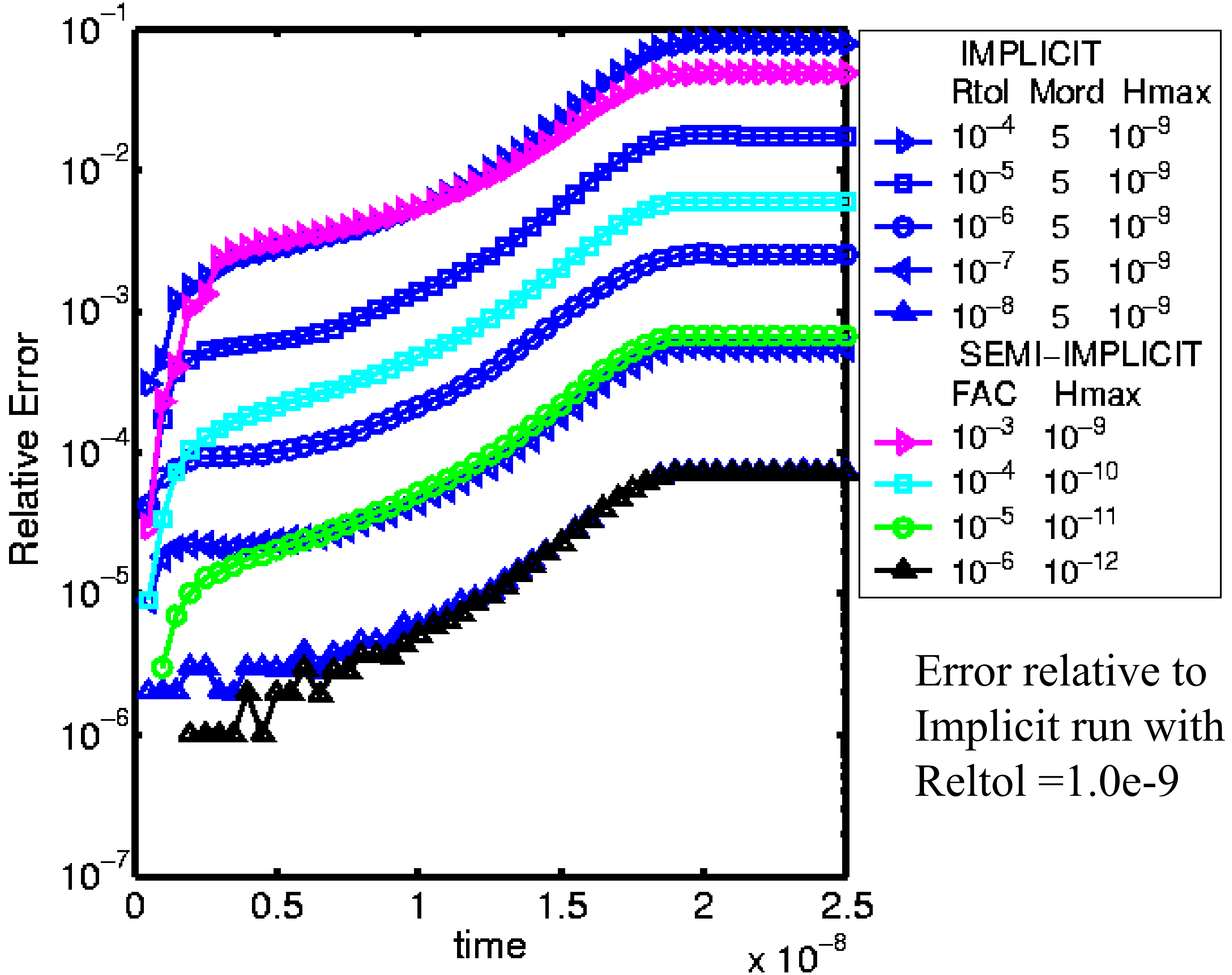
$$(T_M^{n+1})^k \approx (T_M^n)^k + k(T_M^n)^{k-1}\left[\frac{\partial EOS}{\partial T_M}(T_M^n)\right]^{-1}\left(E_M^{n+1} - E_M^n\right)$$

Comparison of Implicit and Semi-Implicit Test Problem

1. 20 X 20 grid, 0.01cm X 0.01 cm
2. Hydrogen, 1.0 gm/cm^3
3. Source "ON" for 2.0e-8 sec
4. LEOS equation-of-state



Relative Error in Material Temperature



Error relative to Implicit run with Reltol =1.0e-9

Implicit and Semi-Implicit Run Times

Implicit

Reltol	NST	Run Time (sec)
1.0e-4	36	0.40
1.0e-5	67	0.92
1.0e-6	125	1.53
1.0e-7	194	2.12
1.0e-8	300	2.90
1.0e-9	513	5.01

Semi-Implicit

FAC	HMAX	NST	Run Time (sec)
1.0e-3	1.0e-9	904	16.5
1.0e-4	1.0e-10	9,754	190.6
1.0e-5	1.0e-11	96,884	1,539.3
1.0e-6	1.0e-12	751,153	1,1744.2

System of Equations with Fuel Density Evolution Equation

Radiation Energy

$$\frac{\partial E_R}{\partial t} = \nabla \cdot \left(\frac{c \nabla E_R}{3 \rho \kappa_R (T_R) + \frac{\left\| \nabla E_R \right\|}{E_R}} \right) + c \rho \kappa_P (T_M) \cdot (a T_M^4 - E_R)$$

Material Energy

$$\frac{\partial E_M}{\partial t} = -c \, \rho \kappa_P (T_M) \cdot (a \, T_M^4 - E_R) + e_r \, \sigma_v \, F^2 \, T_M^5$$

Fuel Density

$$\frac{\partial F}{\partial t} = - \, \sigma_v \, F^2 \, T_M^5$$

CASC

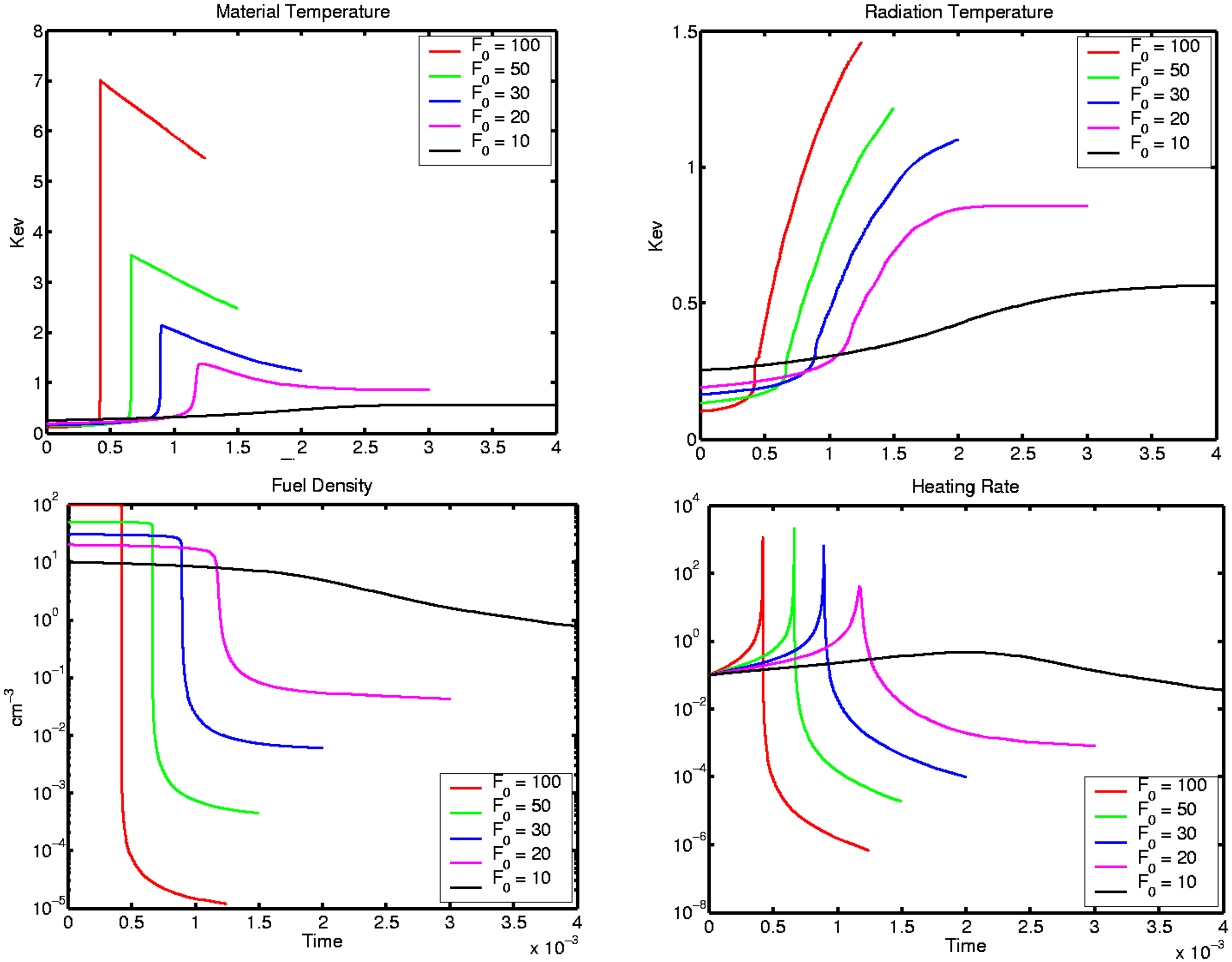
1D Test Problem with Fuel Equation

•Fuel initialized with concentration on right half of domain.

Test Problems

1. Solution Dependence on initial fuel concentration using 20 grid points.
2. Demonstrate effectiveness of Schur complement preconditioner using 20 grid points.
3. Solution profiles near maximum heat rate using 100 grid points
4. Convergence of solution with respect to tolerance parameters using 50 grid points

Solution Dependence on initial fuel concentration using 20 grid points



The Schur complement consists of the diffusion operator plus a diagonal parts

Solutions to systems of the form

$$\mathrm{M}_{\mathrm{Schur}}\, x = \begin{pmatrix} \widetilde{A} & B & 0 \\ C & D & H \\ 0 & N & P \end{pmatrix} x = b$$

Can be written as,

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} S^{-1}(b_1 - B\widetilde{D}^{-1}\widetilde{b}_2) \\ \widetilde{D}^{-1}(\widetilde{b}_2 - Cx_1) \\ P^{-1}(b_3 - Nx_2) \end{pmatrix}$$

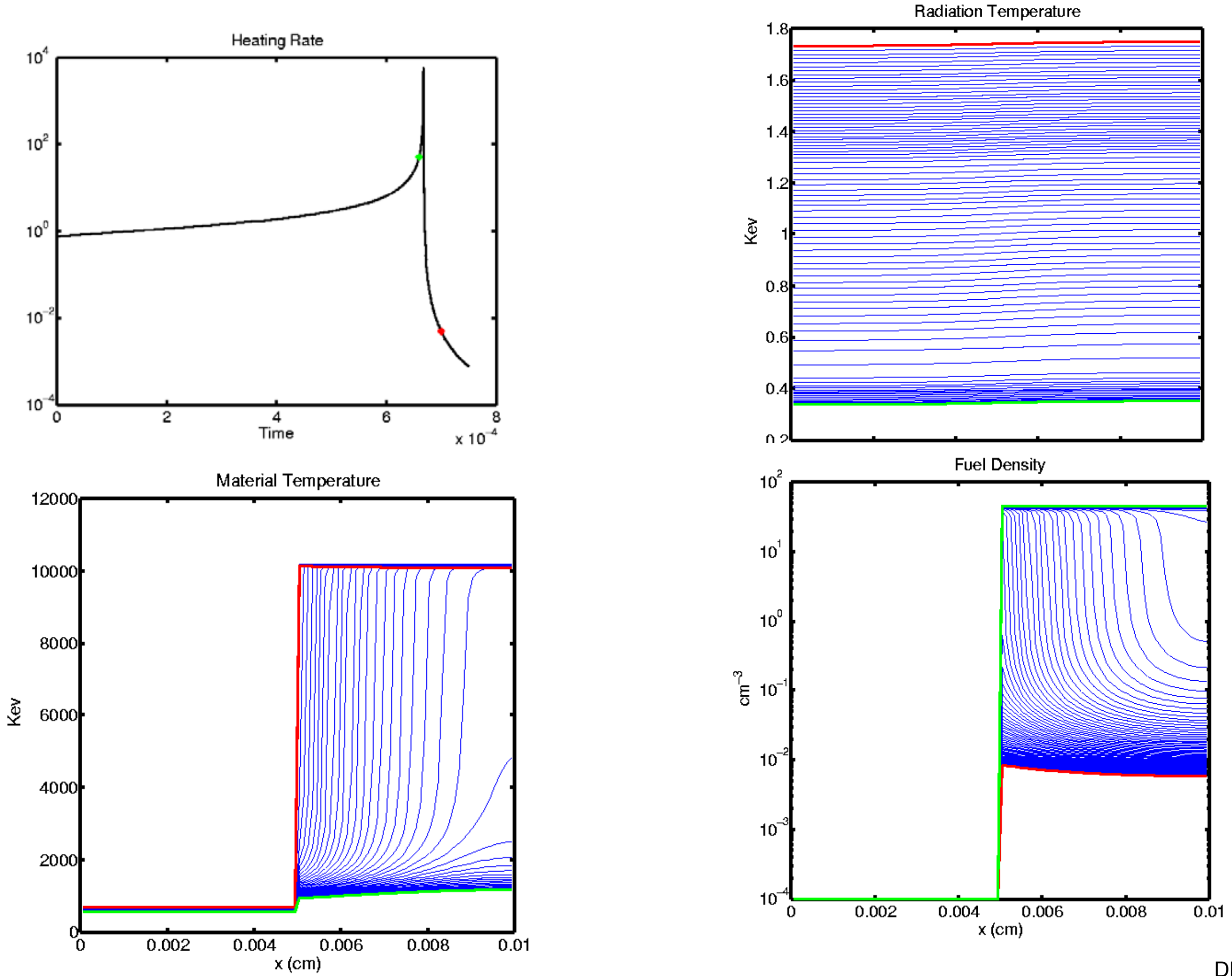
$$S = \widetilde{A} - B\widetilde{D}^{-1}C$$
$$\widetilde{D} = D - HP^{-1}N$$
$$\widetilde{b}_2 = b_2 - HP^{-1}b_3$$

Effectiveness of Schur Complement Preconditioner using 20 grid points

Fuel Density cm^{-3}	Initial Temperature Kev	With PC			Without PC		
		NST	NCFL	Run Time (sec)	NST	NCFL	Run Time (sec)
10	251.20	2,331	0	13.6	5,143	12,768	34.4
30	161.86	5,147	507	13.0	31,298	66,237	180.4
50	132.00	11,078	1983	33.9	46,112	87,909	242.2
100	100.00	Failed			45,022	63,016	200.7

Profiles for 100 grid point case near maximum heating rate.

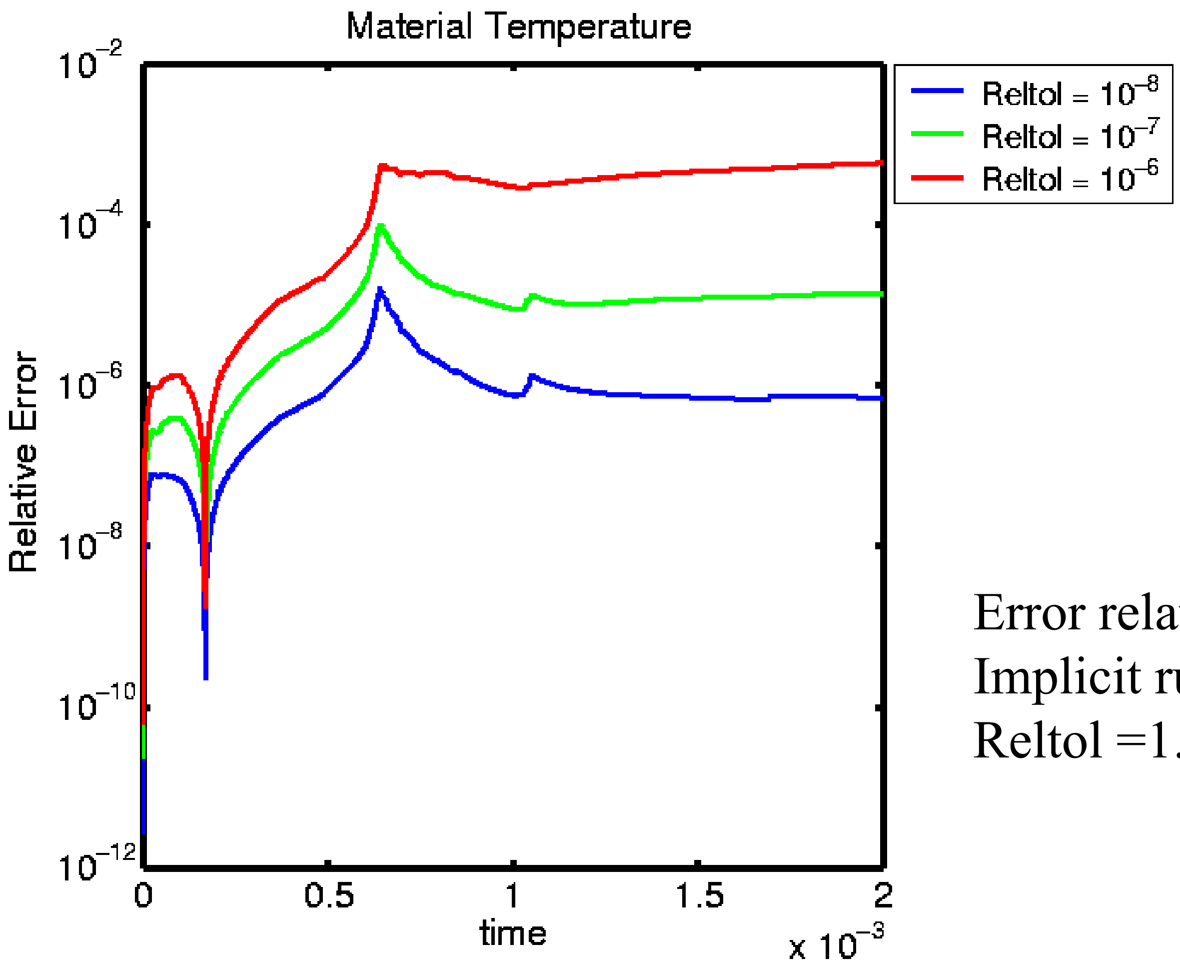
Center Fuel Density = 30.0 cm^{-3}



Convergence with respect to tolerance for 50 grid point 1D problem, Center Fuel Density = 30.0 cm^{-3}

Reltol	Abstol	With Preconditioner			Without Preconditioner		
		NST	NCFL	Run Time (sec)	NST	NCFL	Run Time (sec)
1.0e-6	1.0e-6	2,262	232	17.58	17,795	24,101	255.17
1.0e-7	1.0e-7	5,969	0	20.80	19,654	33,239	184.37
1.0e-8	1.0e-8	13,804	0	68.39	58,784	97,232	714.98
1.0e-9	1.0e-9	33,046	0	103.87	106,341	140,739	866.96

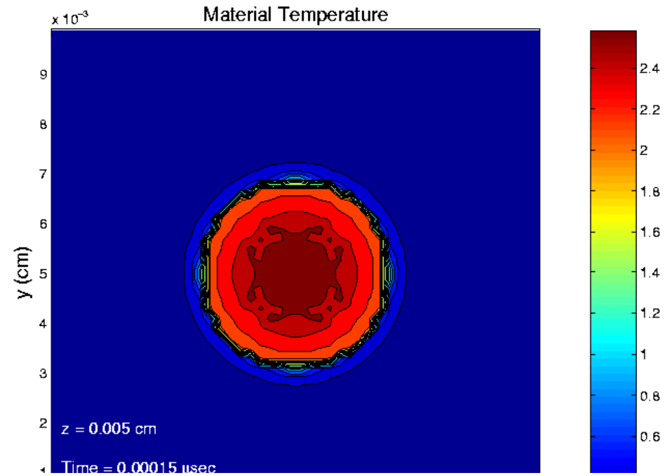
Relative Error in Material Temperature, Center Fuel Density = 30.0 cm^{-3}

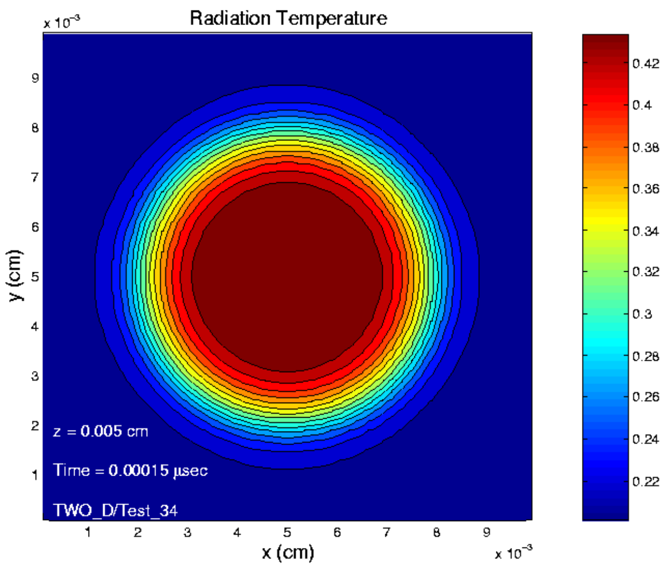


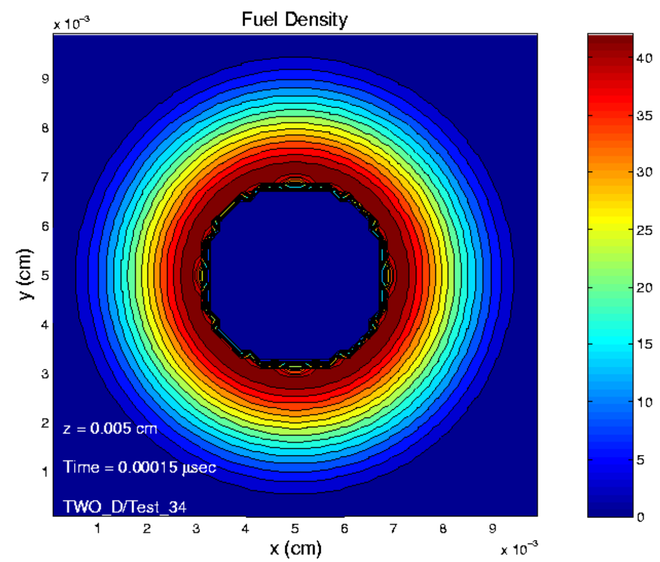
Error relative to Implicit run wth Reltol =1.0e-9

Example of 2D Test Case

- 100 X 100 grid points
- Smooth initial radial profile for fuel
- Number of steps = 23,995
- Run time = 4,251.9 sec







Conclusions

- For two equation system with the new nonlinear source term, the implicit simulations can be an order of magnitude faster than semi-implicit.
- For the new system of equations including the fuel evolution equation, the Schur complement preconditioner can give an order of magnitude reduction in run time.

Future Work

- Understand and correct the failure of the Schur complement preconditioner in the rapid heating test cases.